Structure and Dynamics of Liquids Confined in Silica Nanopores

Anatoli Milischuk [S] and Branka Ladanyi [C]
Colorado State University, Department of Chemistry, Fort Collins, Colorado, U.S.A.
Branka.Ladanyi@colostate.edu

We studied the effects of confinement on static and dynamic properties of liquids including water, acetonitrile, and benzene in amorphous silica nanopores at full hydration and room temperature. The model pores are approximately cylindrical, with diameters ranging from 20 to 40 Å. The filled pores are prepared using grand canonical Monte Carlo simulation and molecular dynamics simulation is used to calculate liquid structure and dynamics. Our studies of dynamics included translational mean squared displacements, orientational time correlations, and survival probabilities in interfacial shells. For benzene and acetonitrile we also studied polarizability anisotropy time correlations that are related to experimentally observed optical Kerr effect response functions, For water we studied hydrogen bond population relaxation and self-intermediate scattering functions related to quasi-elastic neutron scattering (QENS) spectra. We found that there is layering and preferential orientational ordering in the interfacial region. Molecular translational and rotational mobility is reduced in the layers near the interface. However, the radial-axial anisotropy in translational motion largely follows the predictions of a model of free diffusion in a cylinder. The effects of these findings on the experimental observables in QENS and optical Kerr effect will be discussed.